AMENDMENTS TO THE CLAIMS

This listing of claims will replace all prior versions, and listings, of claims in the application.

Claims 1-9 (Canceled)

10. (Currently Amended) A method comprising:

computationally predicting a secondary structure of a protein;

computationally generating a three-dimensional representation of the predicted secondary structure;

optimizing the secondary structure by adjusting dihedral angles ~~using smart moves~~, wherein adjusting the dihedral angles is based on the secondary structure; [[and]]

determining a three-dimensional protein structure by modeling the optimized secondary structure on a topomer model; and

storing the structure on a machine readable medium.

11. (Original) The method of claim 10, wherein said secondary structure is a consensus secondary structure prediction.

12. (Original) The method of claim 10, wherein optimization is performed using a random Monte Carlo method.

13. (Original) The method of claim 12, wherein the random Monte Carlo method is used in conjunction with a localized energy function.

14. (Original) The method of claim 10, wherein said three-dimensional structure model is refined using simulated annealing.

15-21 (Canceled)

22. (Previously Presented) The method of claim 10, wherein the protein secondary structure is predicted by at least one technique selected from the group consisting of Chou-Fasman, GOR (Garnier, Osguthorbe and Robson), PSI-pred, JPRED, Prof, PREDATOR, PHD, ZPRED, nnPredict, BMERC, PSA Server, SSP and PROFsec.

23. (Previously Presented) The method of claim 10, further comprising determining the permissible ranges of phi and psi dihedral bond angles consistent with the predicted secondary structure for each amino acid residue in the protein.

24. (Previously Presented) The method of claim 12, wherein the random Monte Carlo method is performed with or without simulated annealing.

25. (Previously Presented) The method of claim 10, wherein optimization is performed using at least one technique selected from the group consisting of Brownian dynamics, random Monte Carlo, molecular dynamics, simulated annealing, molecular mechanics and energy minimization.

26. (Previously Presented) The method of claim 10, wherein optimization is performed using at least one program selected from the group consisting of AMBER, X-PLOR, INSIGHTII, CHARMM, DISCOVER and GROMOS.

27. (Previously Presented) The method of claim 10, wherein the topomer model is derived using Continuous Configuration Boltzman Biased Direct Monte Carlo Method.

28. (Previously Presented) The method of claim 10, further comprising optimizing the topomer model.

29. (Previously Presented) The method of claim 28, wherein the topomer model is optimized by simulated annealing to minimize free energy.